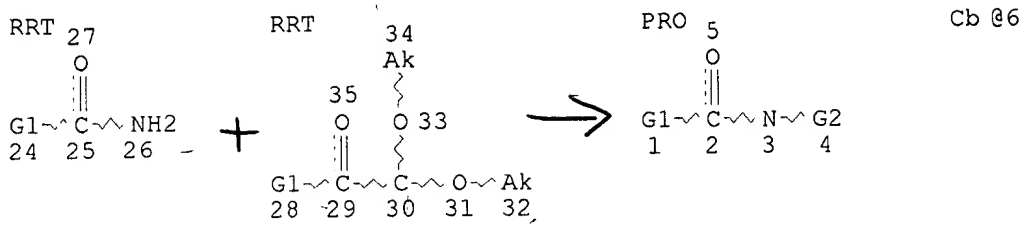
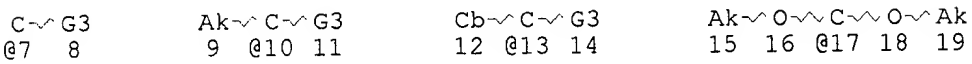
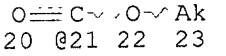
=> d que
L8 STR




VAR G1=H/AK/6
VAR G2=7/10/13
VAR G3=17/21
NODE ATTRIBUTES:
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CONNECT IS E3 RC AT 10
CONNECT IS E3 RC AT 13
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CONNECT IS E3 RC AT 17
CONNECT IS E1 RC AT 19
CONNECT IS E1 RC AT 23
CONNECT IS E3 RC AT 30
CONNECT IS E1 RC AT 32
CONNECT IS E1 RC AT 34
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 6
GGCAT IS UNS AT 12
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M6 C AT 6
ECOUNT IS M6 C AT 12
ECOUNT IS X12 C AT 15
ECOUNT IS X12 C AT 19
ECOUNT IS X12 C AT 23
ECOUNT IS X12 C AT 32
ECOUNT IS X12 C AT 34

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE
L10 1 SEA FILE=CASREACT SSS FUL L8 ( 3 REACTIONS)

=> d ibib abs crd l10

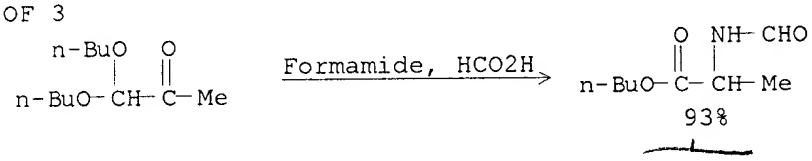
L10 ANSWER 1 OF 1 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 134:178818 CASREACT
TITLE: Process for the preparation of N-(acylamino)acid esters and N-(acylamino)acetals
INVENTOR(S): Paust, Joachim; Ernst, Hansgeorg; Kaczmarek, Reinhard; Jaedicke, Hagen
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: Eur. Pat. Appl., 11 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 1078916 | A1 | 20010228 | EP 2000-115618 | 20000720 |
| EP 1078916 | B1 | 20021211 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| DE 19940641 | A1 | 20010301 | DE 1999-19940641 | 19990826 |
| AT 229495 | E | 20021215 | AT 2000-115618 | 20000720 |
| JP 2001072652 | A2 | 20010321 | JP 2000-252489 | 20000823 |
| CN 1286246 | A | 20010307 | CN 2000-126068 | 20000828 |
| PRIORITY APPLN. INFO.: | | | DE 1999-19940641 | 19990826 |

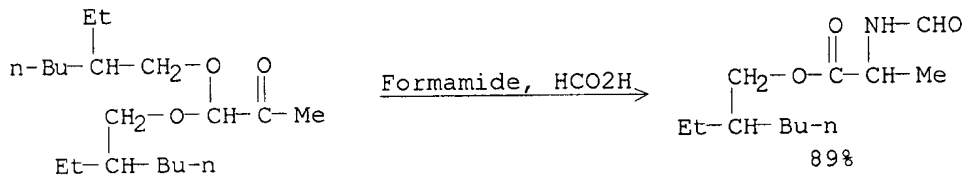
OTHER SOURCE(S): MARPAT 134:178818

AB N-acylamino acid derivs. R1CONHCH(R2)X [R1, R2 = H, C1-12 alkyl, (un)substituted aryl; X = CH(OR3)2, CO2R3; R3 = C1-12 alkyl] (e.g., N-formyl-D,L-alanine Bu ester) are prepd. by the reaction of carboxamides R1CONH2 (e.g., formamide) with a glyoxal monoacetal deriv. R2COCH(OR3)2 (e.g., methylglyoxal dibutylacetal) in the presence of an aliph. carboxylic acid R4CO2H (R4 = C1-12 alkyl) (e.g., formic acid).

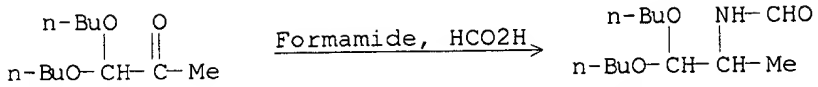
RX(1) OF 3




RX(2) OF 3



RX(3) OF 3




NOTE: lower concn. of formamide and formic acid

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> d que
L1                SCR 273
L2                STR
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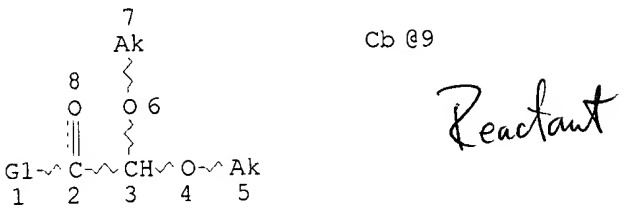


Reactant

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VAR G1=H/AK/9
NODE ATTRIBUTES:
CONNECT IS E1  RC AT    5
CONNECT IS E1  RC AT    7
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT    9
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS X12 C  AT    5
ECOUNT  IS X12 C  AT    7
ECOUNT  IS M6 C  AT    9

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS    9

STEREO ATTRIBUTES: NONE
L3                SCR 278
L4             789 SEA FILE=REGISTRY SSS FUL L1 AND L3 AND L2
L5                STR
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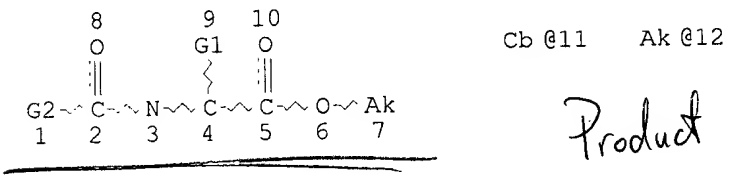


Product

```
VAR G1=AK/11
VAR G2=H/12
NODE ATTRIBUTES:
CONNECT IS E2  RC AT    3
CONNECT IS E3  RC AT    4
CONNECT IS E1  RC AT    7
CONNECT IS E1  RC AT   12
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT   11
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M6 C  AT   11

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   12

STEREO ATTRIBUTES: NONE
L7        485573 SEA FILE=REGISTRY ABB=ON  PLU=ON  NC=1 AND N/ELS AND O>1 NOT
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                (PMS/CI OR RSD/FA)
L9          2959 SEA FILE=REGISTRY SUB=L7 SSS FUL L5
L11          670 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L4(L)(RACT OR RCT OR RGT)/RL
L12         1286 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L9(L)PREP/RL
L13            1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11 AND L12


=> d ibib abs hitstr

L13  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2003 ACS
ACCESSION NUMBER:         2001:152308  HCAPLUS
DOCUMENT NUMBER:          134:178818
TITLE:                    Process for the preparation of N-(acylamino)acid
                          esters and N-(acylamino)acetals
INVENTOR(S):              Paust, Joachim; Ernst, Hansgeorg; Kaczmarek, Reinhard;
                          Jaedicke, Hagen
PATENT ASSIGNEE(S):       BASF Aktiengesellschaft, Germany
SOURCE:                   Eur. Pat. Appl., 11 pp.
                          CODEN: EPXXDW
DOCUMENT TYPE:            Patent
LANGUAGE:                 German
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
     ----------------  ----  --------      ---------------  --------
     EP 1078916        A1    20010228      EP 2000-115618   20000720
     EP 1078916        B1    20021211
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     DE 19940641       A1    20010301      DE 1999-19940641 19990826
     AT 229495         E     20021215      AT 2000-115618   20000720
     JP 2001072652     A2    20010321      JP 2000-252489   20000823
     CN 1286246        A     20010307      CN 2000-126068   20000828
PRIORITY APPLN. INFO.:                    DE 1999-19940641 A  19990826
OTHER SOURCE(S):          CASREACT 134:178818; MARPAT 134:178818
AB   N-acylamino acid derivs. R1CONHCH(R2)X [R1, R2 = H, C1-12 alkyl,
     (un)substituted aryl; X = CH(OR3)2, CO2R3; R3 = C1-12 alkyl] (e.g.,
     N-formyl-D,L-alanine Bu ester) are prepd. by the reaction of carboxamides
     R1CONH2 (e.g., formamide) with a glyoxal monoacetal deriv. R2COCH(OR3)2
     (e.g., methylglyoxal dibutylacetal) in the presence of an aliph.
     carboxylic acid R4CO2H (R4 = C1-12 alkyl) (e.g., formic acid).
IT   86965-96-0P, N-Formyl-D,L-alanine butyl ester 326865-81-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (process for the prepn. of N-(acylamino)acid esters and
        N-(acylamino)acetals)
RN   86965-96-0  HCAPLUS
CN   Alanine, N-formyl-, butyl ester (9CI)  (CA INDEX NAME)
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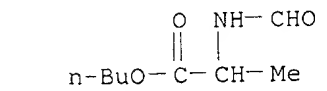

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RN   326865-81-0  HCAPLUS
CN   Alanine, N-formyl-, 2-ethylhexyl ester (9CI)  (CA INDEX NAME)
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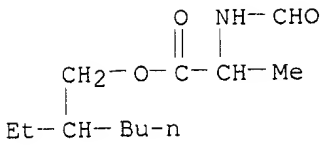
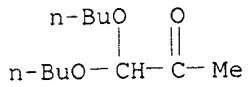
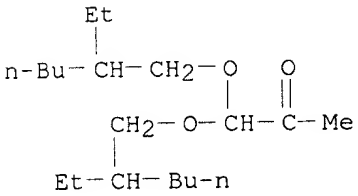


IT **19255-82-4 326865-85-4**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(process for the prepn. of N-(acylamino)acid esters and N-(acylamino)acetals from)
RN 19255-82-4 HCAPLUS
CN 2-Propanone, 1,1-dibutoxy- (9CI) (CA INDEX NAME)



RN 326865-85-4 HCAPLUS
CN 2-Propanone, 1,1-bis[(2-ethylhexyl)oxy]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> d que
L2                SCR 488
L3                STR
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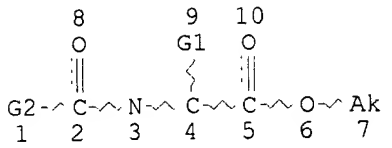


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VAR G1=AK/11
VAR G2=H/12
NODE ATTRIBUTES:
CONNECT IS E2  RC AT   3
CONNECT IS E3  RC AT   4
CONNECT IS E1  RC AT   7
CONNECT IS E1  RC AT  12
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT  11
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M6 C  AT  11

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
L6      1403829 SEA FILE=REGISTRY ABB=ON  PLU=ON  N/ELS AND NC=1 AND O>2 AND
                NRS<2 NOT PMS/CI
L8         3266 SEA FILE=REGISTRY SUB=L6 SSS FUL L2 AND L3
L15             SCR 273
L17             STR
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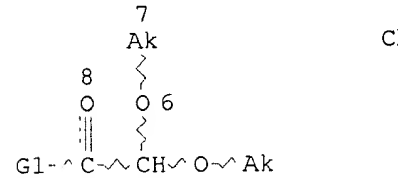


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VAR G1=H/AK/9
NODE ATTRIBUTES:
CONNECT IS E1  RC AT   5
CONNECT IS E1  RC AT   7
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT   9
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS X12 C  AT   5
ECOUNT  IS X12 C  AT   7
ECOUNT  IS M6 C  AT   9

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   9
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STEREO ATTRIBUTES: NONE
L19 SCR 278
L21 789 SEA FILE=REGISTRY SSS FUL L15 AND L19 AND L17
L22 670 SEA FILE=HCAPLUS ABB=ON PLU=ON L21(L)(RACT OR RGT OR RCT)/RL

L23 1727 SEA FILE=HCAPLUS ABB=ON PLU=ON L8(L)PREP/RL
L24 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L22 AND L23

=> d ibib abs hitstr l24 1-3

L24 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:391512 HCAPLUS
DOCUMENT NUMBER: 136:402027
TITLE: Preparation of amino acid derivatives for modulating angiotensin converting enzyme-2 (ACE-2)
INVENTOR(S): Acton, Susan L.; Ocain, Timothy D.; Gould, Alexandra E.; Dales, Natalie A.; Guan, Bing; Brown, James A.; Patane, Michael; Kadambi, Vivek J.; Solomon, Michael; Stricker-Krongrad, Alain
PATENT ASSIGNEE(S): Millennium Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 395 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2002039997 | A2 | 20020523 | WO 2001-US45703 | 20011031 |
| WO 2002039997 | A3 | 20021128 | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

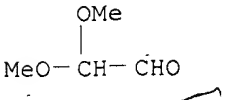
| | | | | |
|---|---|---|---|---|
| AU 2002039454 | A5 | 20020527 | AU 2002-39454 | 20011031 |

PRIORITY APPLN. INFO.:

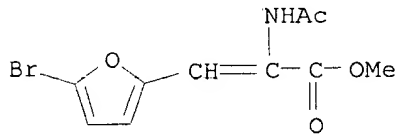
| | | |
|---|---|---|
| US 2000-704216 | A | 20001101 |
| US 2001-870382 | A | 20010529 |
| US 2001-371741P | P | 20011019 |
| WO 2001-US45703 | W | 20011031 |

OTHER SOURCE(S): MARPAT 136:402027
AB ACE-2 modulating compds. Z-A-B-E (Z is a zinc coordinating moiety; E is an enzyme coordinating moiety; A is an auxiliary pocket binding moiety; B is a side chain binding moiety) were prepd. for the treatment of body wt. disorders. Thus, N-[(S)- or (R)-1-carboxy-3-phenylpropyl]-L-leucine was prepd. by the solid-phase method and showed ACE-2 inhibitory activity.
IT **51673-84-8**, Glyoxal dimethyl acetal
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(prepn. of amino acid derivs. for modulating angiotensin converting enzyme-2 (ACE-2))
RN 51673-84-8 HCAPLUS

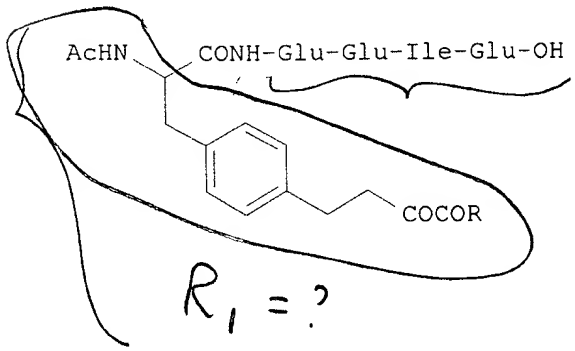
CN Acetaldehyde, dimethoxy- (9CI) (CA INDEX NAME)



IT **429664-62-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of amino acid derivs. for modulating angiotensin converting enzyme-2 (ACE-2))
RN 429664-62-0 HCAPLUS
CN 2-Propenoic acid, 2-(acetylamino)-3-(5-bromo-2-furanyl)-, methyl ester (9CI) (CA INDEX NAME)



L24 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1996:545197 HCAPLUS
DOCUMENT NUMBER: 125:301538
TITLE: .alpha.-Dicarbonyls as "non-charged" arginine-directed affinity labels. Novel synthetic routes to .alpha.-dicarbonyl analogs of the PP60c-src SH2 domain-targeted phosphopeptide Ac-Tyr(OPO3H2)-Glu-Glu-Ile-Glu
AUTHOR(S): Mehrotra, Mukund M.; Sternbach, Daniel D.; Ridriguez, Marc; Charifson, Paul; Berman, Judd
CORPORATE SOURCE: Glaxo Wellcome Res., Research Triange Park, NC, 27709, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(16), 1941-1946
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

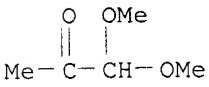


I

AB Title phosphopeptide is a potent inhibitor of pp60c-src SH2 domain mediated phosphoprotein interactions (IC50 .ltoreq. 0.5 .mu.M), but lacks cell permeability. The syntheses of its less charged analogs I (R = Me, H) are described, in which the arginine-binding phosphate group has been substituted with uncharged .alpha.-dicarbonyl moieties. The chem. described here may be of general use for the synthesis of other .alpha.-dicarbonyl compds.

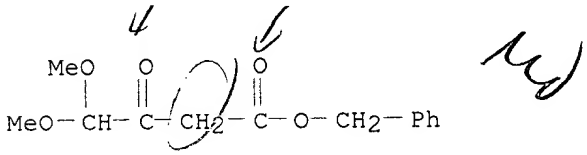
IT **6342-56-9**, Pyruvic aldehyde dimethylacetal
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(synthesis of dicarbonyl analogs of PP60c-src SH2 domain-targeted phosphopeptide)

RN 6342-56-9 HCAPLUS
CN 2-Propanone, 1,1-dimethoxy- (9CI) (CA INDEX NAME)



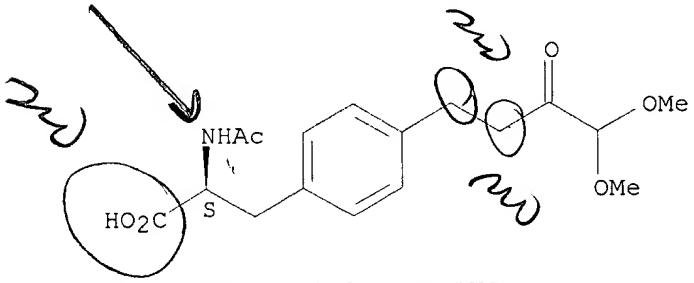
IT **182617-55-6P 182617-58-9P 182617-59-0P 182617-60-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation); RACT (Reactant or reagent)**
(synthesis of dicarbonyl analogs of PP60c-src SH2 domain-targeted phosphopeptide)

RN 182617-55-6 HCAPLUS
CN Butanoic acid, 4,4-dimethoxy-3-oxo-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 182617-58-9 HCAPLUS
CN L-Phenylalanine, N-acetyl-4-(4,4-dimethoxy-3-oxobutyl)- (9CI) (CA INDEX NAME)

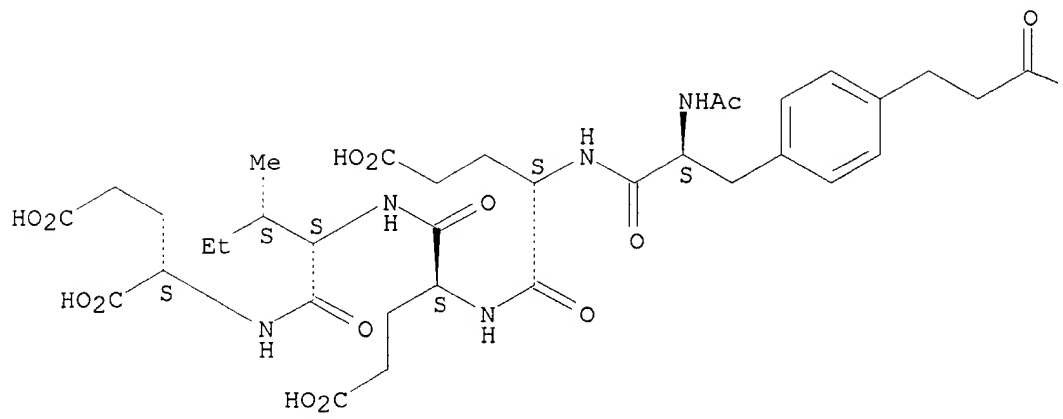
Absolute stereochemistry.



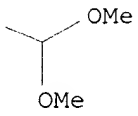
RN 182617-59-0 HCAPLUS
CN L-Glutamic acid, N-[N-[N-[N-[N-acetyl-4-(4,4-dimethoxy-3-oxobutyl)-L-phenylalanyl]-L-.alpha.-glutamyl]-L-.alpha.-glutamyl]-L-isoleucyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

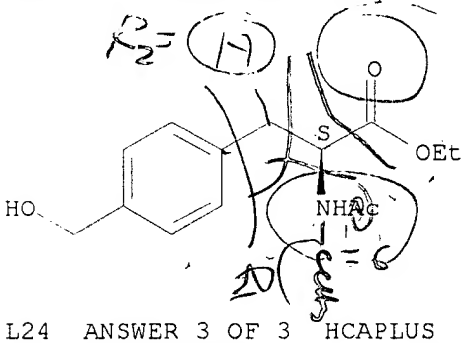


PAGE 1-B



RN 182617-60-3 HCAPLUS
CN L-Phenylalanine, N-acetyl-4-(hydroxymethyl)-, ethyl ester (9CI) (CA INDEX NAME)

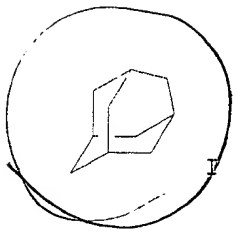
Absolute stereochemistry.



L24 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2003 ACS

| | |
|---|---|
| ACCESSION NUMBER: | 1984:51141 HCAPLUS |
| DOCUMENT NUMBER: | 100:51141 |
| TITLE: | New syntheses and reactions in the adamantane series |
| AUTHOR(S): | Stetter, Hermann; Mayska, Paul; Wiessner, Ulrich |
| CORPORATE SOURCE: | Inst. Org. Chem., Rhein.-Westf. Techn. Hochsch. Aachen, Aachen, Fed. Rep. Ger. |
| SOURCE: | Forschungsberichte des Landes Nordrhein-Westfalen (1982), 3095, 128 pp. CODEN: FLNWAR; ISSN: 0367-2492 |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | German |

GI



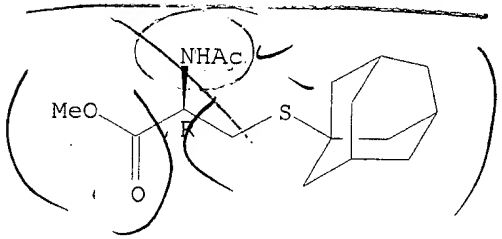
AB An exhaustive investigation was carried out of the reactions of adamantane (I) derivs., including the use of 1-adamantyl, 1-adamantylthio, and 1-adamantylsulfinyl groups as protective groups in amino acid and peptide synthesis.

IT **88458-86-0P 88458-87-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. and deprotection and sapon. of)

RN 88458-86-0 HCAPLUS

CN L-Cysteine, N-acetyl-S-tricyclo[3.3.1.13,7]dec-1-yl-, methyl ester (9CI) (CA INDEX NAME)

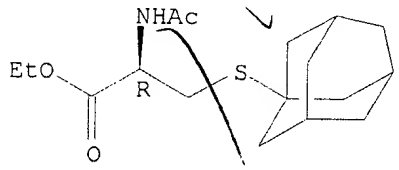
Absolute stereochemistry.




RN 88458-87-1 HCAPLUS

CN L-Cysteine, N-acetyl-S-tricyclo[3.3.1.13,7]dec-1-yl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.




IT **5344-23-0**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(reaction of, with aminoadamantane)

RN 5344-23-0 HCAPLUS

CN Acetaldehyde, diethoxy- (9CI) (CA INDEX NAME)